CHARGE NUMBER: 0108

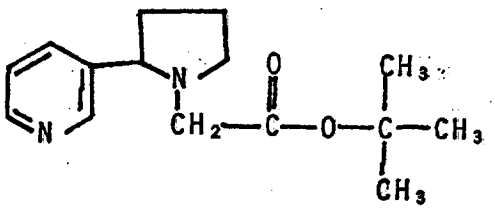
PROGRAM TITLE: Mechanism for Smoke Formation

PERIOD COVERED: April 1 - May 1, 1980

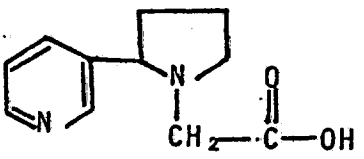
PROJECT LEADER: R. A. Kornfeld

DATE OF REPORT: May 6, 1980

The pyrolytic yields of nicotine and myosmine were calculated at several temperatures for the thermolysis of t-butyl 2-(3-pyridyl)-pyrrolidinylacetate (A) and 2-(3-pyridyl)pyrrolidinyl acetic acid (B). Both of these compounds were synthesized by G. Chan as potential nicotine release agents. Preliminary information for the pyrolysis of these two compounds was reported last month.



A



B

The molar percent yields of both nicotine and myosmine from the t-butyl ester (A) were low. Up to 500°C nicotine was produced at the 0.2-0.3% level while myosmine yields were 4-5%. At 550°C the nicotine and myosmine yields were 1% and 15% respectively. The formation of nicotine and myosmine from the acid (B) are shown below. The molar percent yields of nicotine remain essentially constant until about 500°C. At temperatures above 500°C, the yield decreases. While myosmine does not produce a detectable peak until 400°C, this compound's yield increases dramatically until it approaches the amount of nicotine present.

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Source: https://www.industrydocuments.ucsf.edu/docs/nljm0000

Temperature (°C)	Pyrolytic Molar Nicotine	Yield from B of Myosmine~
250	12%	N.D.
300	13%	N.D.
350	13%	N.D.
400	13%	5%
450	13%	12%
500	18%	16%
550	8%	6%
600	1%	3%

N.D. = not detected

Reasons for the low nicotine and relatively high myosmine yields are being pursued!

In addition to the installation of the capillary inlet system reported last month, the Hewlett-Packard gas chromatograph can now operate in a sample split or splitless mode. Several test flavor mixtures, smoke samples, and fractions of a Browning reaction mixture (in cooperation with M. Edmonds) were chromatographed.[2]

Several furan derivatives (2-furfural, 2-furoic acid and 5-hydroxymethyl 2-furfural) were pyrolyzed alone and copyrolyzed with ammonium carbonate at 600°C and 800°C. Based solely on GC retention data, several pyridines were tentatively identified. The only furan compound to show even a trace of pyrazines at 600°C is 2-furoic acid. All co-pyrolyzates show a trace of methyl pyrazine at 800°C. None of these co-pyrolyses produced significant amounts of simple pyrazines. Copyrolyses with another nitrogen source, glycine or alanine, will be pursued during the next month.[3]

It was found that cigarettes wrapped with paper containing added phosphate yielded 50% more CO when compared to the same cigarettes using untreated or citrate treated paper.[4] In an attempt to determine if this observation could be explained via a pyrolysis mechanism; phosphate treated, citrate treated, and untreated cigarette papers were pyrolyzed at 800°C and the amount of CO was quantitated by gas chromatography. It was found that the untreated and treated papers yielded the same amount of CO. However, a comparison with the citrate treated (Monitor) paper showed a 15% decrease in CO yield!

A mixture[5] of 2'-methyl-nicotine (C) and 2',6-dimethylnicotine (D) was analyzed by computerized GC/MS. The mass spectra were consistent with the proposed structure.[6]

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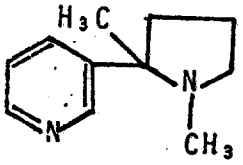
Source: https://www.industrydocuments.ucsf.edu/docs/nljm0000



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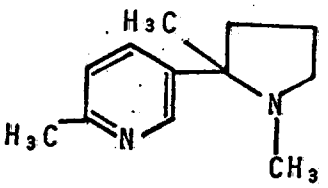

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Pyrolysis/GC/MS analyses for the materials evaluation program continue. The following memoranda were issued:

"Pyrolysis GC/MS of Samples Z9ZF-A&C", memo to Mr. R. D. Carpenter from D. F. Magin, April 17, 1980

"Pyrolysis GC/MS of Sample Z9YW", memo to Mr. R. D. Carpenter from D. F. Magin, May 1, 1980.

Rich Kornfeld

References:

1. L. Brown 7223
2. F. Greene 7336
3. J. Kang 7262
4. R. Newman 6549 (Project 2501)
5. H. Secor sample number 7386-149C
6. D. Magin 7474

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